

The influence of the elementary charge on the canonical quantization of LC -circuits

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Abstract

In this paper one deals with the quantization of mesoscopic LC -circuits under the influence of an external time dependent voltage. The canonically conjugated variables, such as given by the electric charge and the magnetic flux, get established by resorting to the hamiltonian equations of motion provided by both Faraday and Kirchhoff laws. This time the discretization of the electric charge is accounted for, so that magnetic flux operators one looks for should proceed in terms of discrete derivatives. However, the flux operators one deals with are not Hermitian, which means that subsequent symmetrizations are in order. The eigenvalues characterizing such operators can be readily established in terms of twisted boundary conditions. Besides the discrete Schrödinger equation with nearest-neighbor hoppings, a nontrivial next nearest neighbor generalization has also been established. Such issues open the way to the derivation of persistent currents in terms of effective k -dependent Hamiltonians. Handling the time dependent voltage within the nearest neighbor description leads to the derivation of dynamic localization effects in L -ring configurations, such as discussed before by Dunlap and Kenkre. The onset of the magnetic flux quantum has also been discussed in some more detail.

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I. INTRODUCTION

The increasing miniaturization of electric mesoscopic devices attains a stage in which the length scale of the LC -system becomes smaller than the so called phase coherence length, which stands for the length scale characterizing quantum interference devices. This means that the quantization of the LC -circuit is in order [1]. We shall then proceed by applying the canonical quantization, now by selecting canonically conjugated variables one deals with in an appropriate manner, such as given by the electric charge Q and the rescaled magnetic Φ/c [2]. For this purpose we have to remind that the energy terms concerning the capacitance C and the inductance L are given by $Q^2/2C$ and $\Phi^2/2Lc^2$, respectively. Accordingly, one deals with the total Hamiltonian

$$H(Q, \Phi/c) = \frac{\Phi^2}{2Lc^2} + \frac{Q^2}{2C} - QV_s(t) \quad (1)$$

in which the influence of an external time dependent voltage has also been included. Accordingly, the Hamiltonian equations of motion are given by $\dot{\Phi} = IL\dot{Q}$ and

$$U = V_s(t) - \frac{d}{dt} \left(\frac{\Phi}{c} \right) \quad (2)$$

where $I = dQ/dt$ and $U = Q/C$. This supports the selection of canonically conjugated variables just done above. Just remark that (2) encompasses both Faraday's law of induction and the second law of Kirchhoff.

So, one gets faced with the canonical commutation relation

$$[Q_{op}, \Phi_{op}] = i\hbar c, \quad (3)$$

where by now Q_{op} and Φ_{op} denote quantum-mechanical observables concerning the electric charge and the magnetic flux, respectively. In this context Eq.(3) is responsible for the quantization of the LC -circuit.

Next let us look for a solution of Eq.(3), now by accounting for the existence of an elementary charge, say $q_e = e = 1.60217733 \times 10^{-19}C$, with the understanding that the charge of the electron is $-e$. We then have to say that the charge Q is a discrete one if $Q = nq_e$, where n denotes an integer. Our next task is to perform the quantization of the LC -circuit referred to above in terms of the right-hand and left-hand discrete derivatives Δ

and ∇ for which

$$\Delta f(n) = f(n+1) - f(n) \quad \text{and} \quad \nabla f(n) = f(n) - f(n-1) \quad (4)$$

in which case $\Delta^+ = -\nabla$ and $\Delta\nabla = \Delta - \nabla$. We have to say that the n -integer is provided by the eigenvalue equation [3]

$$Q_{op} | n \rangle = Q | n \rangle \quad (5)$$

where $Q = nq_e$. Disregarding for the moment Eq. (5), leads us to say that the canonical commutation relation (3) exhibits the solution

$$\Phi_{op} = -i\hbar c \frac{\partial}{\partial Q} = -i \frac{\hbar c}{q_e} \frac{\partial}{\partial n} \quad (6)$$

in so far as Q is a continuous variable. We have to remark that the quotient $\delta\Phi = \hbar c/q_e = h/2q_e(c/2\pi)$ in (6) serve as a candidate for the magnetic flux quantum, but further clarifications remain desirable. Indeed, the magnetic flux quantum, say ϕ_0 , is registered in data tables of fundamental constants as $\phi_0 = h/2e = 2.06783372 \cdot 10^{-15} \text{Wb}$, in which case $\delta\Phi/\phi_0 = c/2\pi$. Moreover, the magnetic flux quantum, in CGS-units, such as used in connection with the Aharonov-Bohm effect reads $\phi_A = hc/q_e$. Of course, ϕ_0 differs both from $\delta\Phi$ and ϕ_A , which indicates that a safe theoretical derivation of the magnetic flux quantum is in order.

II. MAGNETIC FLUX-STRUCTURES AND MAGNETIC ENERGIES

The derivation of the discrete counterpart of (6) requires a little bit more attention. Indeed, in this case one gets faced with two non-Hermitian realizations of the magnetic flux-operator, say [4]

$$\Phi_{op}^{(1)} = \frac{-i\hbar c}{q_e} \nabla \quad (7)$$

and

$$\Phi_{op}^{(2)} = \frac{-i\hbar c}{q_e} \Delta = (\Phi_{op}^{(1)})^+. \quad (8)$$

Accordingly, the symmetrized Hermitian magnetic flux operator is given by

$$\Phi_{sym} = \frac{-i\hbar c}{2q_e} (\Delta + \nabla). \quad (9)$$

Then the eigenvalues of such operators should provide realizations of a quantized magnetic flux. In addition, the Hermitian flux operator Φ_{sym} yields a symmetrized magnetic energy via

$$H_{sym} = H_{NNN} = \frac{1}{2Lc^2} \Phi_{sym}^2 = -\frac{\hbar^2}{8Lq_e^2} (\Delta + \nabla)^2, \quad (10)$$

which is responsible for next nearest-neighbor (NNN) hoppings.

In addition, we have to look for an Hermitian magnetic energy operator like

$$H_m = H_{NN} = \frac{1}{2Lc^2} (\Phi_{op}^{(1)})^+ \Phi_{op}^{(1)} = -\frac{\hbar^2}{2Lq_e^2} (\Delta - \nabla), \quad (11)$$

which is provided by a different kind of symmetrization and which is responsible for nearest-neighbor (NN) hoppings. So one gets faced with two competing Hermitian realizations, i.e. with H_{NN} and H_{NNN} , proceeding solely in a direct connection with the underlying symmetrization. In other words we have to account for an actual sensitivity with respect to the symmetrization path, which looks interesting from a theoretical point of view. We have also to mention that under the discretization of the electric charge the canonical commutation relation (3) gets modified as

$$[Q_{op}, \Phi_{sym}] = -i\hbar c \left(1 - \frac{q_e^2 L}{\hbar^2} H_m \right) \quad (12)$$

which can be viewed as a deformed algebraic structure. Note that such structures have received much attention during the last 2 – 3 decades of the former century [5].

The energy dispersion laws characterizing H_{NN} and H_{NNN} , say $E_{NN}(k)$ and $E_{NNN}(k)$, can also be readily established. One obtains

$$E_{NN}(k) = -\frac{\hbar^2}{Lq_e^2} (\cos k - 1) \quad (13)$$

and

$$E_{NNN}(k) = \frac{\hbar^2}{2Lq_e^2} \sin^2 k \quad (14)$$

which are both even functions of the k -parameter, as one might expect.

III. REVISITING THE DISCRETE NN- AND NNN- SCHRÖDINGER EQUATIONS OF THE LC -CIRCUIT

Next let us discuss the Schrödinger equation of the LC -circuit by resorting to the magnetic energy H_m such as written down above in (11). This equation exhibits the general form

$$H_m | \Psi \rangle = i\hbar \frac{\partial}{\partial t} | \Psi \rangle \quad (15)$$

which will be handled in terms of the wavefunction

$$\varphi_m(t) = \langle m | \Psi \rangle. \quad (16)$$

where m is an integer. This leads to the second order discrete equation with NN-hoppings

$$-\frac{\hbar^2}{2Lq_e^2}(\varphi_{m+1} + \varphi_{m-1}) + \left(\frac{q_e^2}{2C}m^2 - mq_e V_s(t) + \frac{\hbar^2}{Lq_e^2} \right) \varphi_m = i\hbar \frac{\partial}{\partial t} \varphi_m, \quad (17)$$

which looks like a perturbed harmonic oscillator on the discrete space. One realizes that the constant \hbar^2/Lq_e^2 -term in (17) can be gauged away. In addition, (17) shows that the NN overlap integral is given by $J_{NN} = -\hbar^2/2Lq_e^2$. Accounting for NNN-hoppings, one realizes that (17) gets replaced by

$$-\frac{\hbar^2}{8Lq_e^2}(\varphi_{m+2} + \varphi_{m-2}) + \left(\frac{q_e^2}{2C}m^2 - mq_e V_s(t) + \frac{\hbar^2}{4Lq_e^2} \right) \varphi_m = i\hbar \frac{\partial}{\partial t} \varphi_m, \quad (18)$$

by virtue of (10). One sees that J_{NN} gets modified as $J_{NNN} = -\hbar^2/8Lq_e^2$. It is understood that such issues have to be viewed as first principles results.

Neglecting the term quadratic in the discrete coordinate m , it can be easily verified that the Fourier transform

$$\varphi_m = \frac{1}{2\pi} \int dk C_k(t) \exp(imk). \quad (19)$$

leads to the conversion of (17) into

$$\left(-\frac{\hbar^2}{Lq_e^2} \cos k - iq_e V_s(t) \frac{\partial}{\partial k} \right) C_k(t) = i\hbar \frac{\partial}{\partial t} C_k(t), \quad (20)$$

which works in the k -representation. A similar transformation can also be done for (18). However, it should be remarked that the Hamiltonian characterizing (20) is not Hermitian for

realistic systems for which $V_s(t) \neq 0$, unless one considers a time lattice in which $V_s(t) = 0$. Now we have to say that more detailed transformations providing equivalent Hamiltonians which are both k - and flux-dependent have been discussed [6]. We shall then apply this latter approach to the study of the magnetic flux quantum, now by accounting in an explicit manner for the k -parity of the Hamiltonian. Proceeding in this manner opens the way to a proper derivation of the magnetic flux quantum ϕ_0 one looks for. For this purpose one resorts to the shifted Fourier-transform

$$u(k, t) = \sum_{n=-\infty}^{n=\infty} C_n(t, k) \exp in \left(k + \frac{q_e \Phi_e}{\hbar c} \right) \quad (21)$$

in which case (17) gets converted into

$$H_{eff}(k, \Phi) C_n(t, k) = i\hbar \frac{\partial}{\partial t} C_n(t, k), \quad (22)$$

where

$$H_{eff}(k, \Phi) = -\frac{q_e^2}{2C} \frac{\partial^2}{\partial k^2} + \frac{\hbar^2}{q_e^2 L} \left(1 - \cos \left(k + \frac{q_e \Phi_e}{\hbar c} \right) \right), \quad (23)$$

denotes the effective k -dependent Hamiltonian and where Φ_e stands for the external flux. The persistent current is then given by

$$I_k(t) = -c \frac{\partial H_{eff}}{\partial \Phi_e} = -\frac{\hbar}{q_e L} \sin \left(k + \frac{q_e \Phi_e}{\hbar c} \right). \quad (24)$$

Assuming that the effective Hamiltonian displayed above is an even function of k , yields the flux quantization rule one looks for as

$$\frac{q_e \Phi_e}{\hbar c} = \frac{n}{2}, \quad (25)$$

where n is an integer. This shows that the magnetic flux quantum is given precisely by $\Phi_0 = \hbar c / 2q_e$, with the understanding that the c -factor is reminiscent to CGS-units.

IV. APPLYING MAGNETIC FLUX OPERATORS IN TERMS OF TWISTED BOUNDARY CONDITIONS

The motion of an electron on a 1-D ring threaded by an external magnetic flux Φ_e is characterized by the twisted boundary condition [7]

$$\varphi(x + L) = \exp 2\pi i (\beta + n) \varphi(x), \quad (26)$$

in which $n = 0, \pm 1, \pm 2, \dots$ and $\beta = \Phi_e / \Phi_0$. The electron coordinate along the ring and the ring circumference are denoted by x and L , respectively. One has

$$\Delta\varphi(x) = \varphi(x + L) - \varphi(x) = 2i \exp i\pi (\beta + n) \sin \pi (\beta + n) \varphi(x), \quad (27)$$

so that

$$\Phi_{op}^{(2)}\varphi(x) = \frac{-i\hbar c}{q_e}\Delta\varphi(x) = \frac{2\hbar c}{q_e} \exp(i\pi(\beta + n)) \sin(\pi(\beta + n))\varphi(x). \quad (28)$$

Proceeding in a similar manner one finds

$$\Phi_{sym}\varphi(x) = \frac{\hbar c}{q_e} \sin(2\pi(\beta + n))\varphi(x). \quad (29)$$

We can then say that the eigenvalues of the flux operators one deals with can be established actually in terms of Eq.(26), which serves for a deeper understanding. However, further clarifications remain desirable.

V. CONCLUSIONS

In this paper the canonical quantization of the mesoscopic LC -circuit has been discussed under specific conditions concerning the discrete spectrum of the electric charge as well as the influence of an external time dependent voltage. This amounts to formulate the magnetic flux operator in terms of right- and left-hand discrete derivatives, as shown by (7) and (8). Such operators are not hermitian owing to the very incorporation of discrete derivatives, but a hermitian realization can be readily established by resorting to a subsequent symmetrization, such as displayed in (9). The eigenvalues of such operators have been established by resorting to twisted boundary conditions. A deformed canonical commutation relation between electric charge and magnetic flux such as given by (12) has also been derived. This is a nontrivial result which deserves further attention from the theoretical point of view. The derivation of the discrete Schrödinger equations of the LC -circuit, say (17) and (18), by accounting for the magnetic energy operators $H_m = H_{NN}$ and $H_{sym} = H_{NNN}$, should also be mentioned. Moreover, these equations exhibit the attributes of first-principles

descriptions as they provide both the hopping configurations as well as the corresponding overlap integrals. And last but not at least a safe derivation of the magnetic flux quantum has also been established as shown by Eq.(25). To this aim one should deal with effective Hamiltonians which are even functions of the wavenumber k .

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